Ferromagnetic Kondo effect in a triple quantum dot system

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We propose that a simple device of three laterally-coupled quantum dots, the central one contacted by metal leads, can realize the ferromagnetic Kondo model, which is characterized by interesting properties like a non-analytic inverted zero-bias anomaly and an extreme sensitivity to a magnetic field. Furthermore, by tuning the gate voltages of the lateral dots, this device may allow to study the transition from ferromagnetic to antiferromagnetic Kondo effect, a simple case of a Berezinskii-Kosterlitz-Thouless transition. We model the device by three coupled Anderson impurities that we study by numerical renormalization group. We calculate the single-particle spectral function of the central dot, which at zero frequency is proportional to the zero-bias conductance, across the transition, both in the absence and in the presence of a magnetic field.

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In spite of its simplicity – a magnetic impurity embedded in a conduction bath – the Kondo model exhibits rich many-body physics[1] that continues to attract scientific interest in a variety of contexts. It is common to distinguish between Kondo models with Fermi-liquid properties *a' la* Noziéres[2] from those that instead display non-analytic, hence non-Fermi-liquid, behavior as function of state variables, and which include under- and over-screened Kondo models[1, 3, 4] as well as clusters of magnetic impurities in particular circumstances[5–7]. Non-Fermi liquid properties are not common in traditional magnetic alloys,[8] where the metal hosts generally possess enough scattering channels that can perfectly screen the magnetic impurity. They may instead be realized in confined scattering geometries such as a quantum dot or a magnetic atom/molecule contacted by metal leads. Indeed, by means of such devices there are already many experimental realizations of exotic non-Fermi-liquid Kondo models, see e.g. Refs. [9], [10], [11] and [12].

One case, however, which so far remains elusive is the ferromagnetic Kondo model (FKM)[13] – where the impurity and the conduction electrons are coupled ferromagnetically – except for its indirect manifestation in the under-screened Kondo effect.[3, 9] It has been proposed that the so-called giant moments induced by $3d$ transition metal impurities diluted in $4d$ transition metals may actually be a manifestation of FKM,[14] but experiments that could pin it down are still lacking. This is unfortunate since the FKM is the simplest example of non-Fermi liquid behavior; at low temperature the impurity spin behaves essentially as a free local moment apart from logarithmic singularities.[13, 15]

Here we present a possible realization of a FKM by means of three laterally-coupled quantum dots. We also discuss the appealing possibility of crossing the Berezinskii-Kosterlitz-Thouless (BKT) phase transition from ferromagnetic to antiferromagnetic Kondo effect,

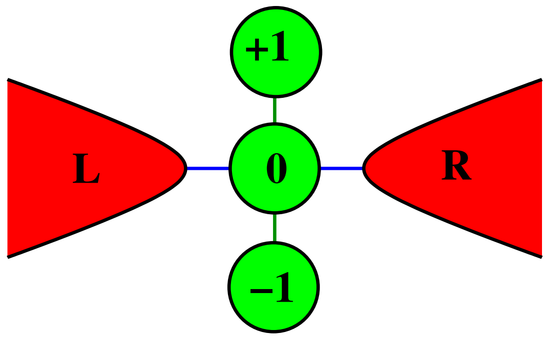

FIG. 1. (Color online) A schematic representation of our device described by Eq. 1, with three quantum dots (in green). Only the central one, labelled as 0, is attached to metallic leads (in red).

whose spectral weight anomaly change we study here by means of numerical renormalization group (NRG)[16–18] in a toy-model for the device.

Our *gedanken* (but entirely feasible)[19, 20] set-up, schematically shown in fig. 1, consists of three quantum dots, labelled as ±1 and 0 in the figure, with the central one contacted by two metal leads, R and L. We model the isolated three-dot device with a Hamiltonian

$$\mathcal{H} = \sum_{i=-1}^{+1} \left(\epsilon_i n_i + \frac{U_i}{2} \left(n_i - 1\right)^2 \right) - \sum_{\sigma} \left(t_- \, c^\dagger_{-1\sigma} c_{0\sigma} + t_+ \, c^\dagger_{0\sigma} c_{+1} + H.c. \right), \qquad (1)$$

where we keep just one orbital per dot, U_i are the charging energies, and the dots are mutually coupled by single-particle tunneling. As usual, we shall assume non-interacting leads, coupled to the central dot 0 by tunneling. For convenience, we also assume equivalent R and L leads , so that only their symmetric combination matters in the linear response regime of interest to us. Particle-

hole symmetry is also assumed. The lead-dot tunneling is thus parametrized by a single quantity, the hybridization width $\Gamma = \pi \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2\, \delta(\epsilon_{\mathbf{k}})$, where $\epsilon_{\mathbf{k}}$ is the energy and $V_{\mathbf{k}}$ the tunneling amplitude into the dot of the symmetric $L+R$ combination of the lead electrons at momentum $\mathbf{k}$.

We further assume that each dot is brought by gate voltage in the Coulomb blockade regime with a single unpaired electron, i.e. $\epsilon_i \simeq 0$ and $t_\pm \ll U_i$, $\forall i$. In this limit, the isolated trimer behaves like a three-site Heisenberg model described by an effective Hamiltonian

$$\mathcal{H}_{\text{eff}} = J_+\, \mathbf{S}_0 \cdot \mathbf{S}_{+1} + J_-\, \mathbf{S}_0 \cdot \mathbf{S}_{-1}, \tag{2}$$

with positive $J_\pm$, where $\mathbf{S}_i$, $i = 0, \pm 1$, are spin-1/2 operators residing on the corresponding dots. The ground state of (2) has total spin 1/2 and explicitly reads

$$|\,\text{GS}, \sigma\rangle = \cos\theta\ |\,\text{O}, \sigma\rangle - \sin\theta\ |\,\text{E}, \sigma\rangle, \tag{3}$$

where $\sigma =\uparrow, \downarrow$ is the z-component of the total spin, and $\tan 2\theta = \sqrt{3}\,\big(J_+ - J_-\big)/\big(J_+ + J_-\big)$. In Eq. (3), $|\,\text{O}, \sigma\rangle$ is the state, odd by inversion through dot 0, obtained by coupling dots $+1$ and -1 into a triplet and coupling the latter to dot 0 to form a spin 1/2. Vice versa, $|\,\text{E}, \sigma\rangle$ is the state, even by reflection, obtained by coupling dots $+1$ and -1 into a singlet, leaving a free spin-1/2 on dot 0.

If on dot 0 the electron is removed or one more electron is added through the leads, the trimer ends up in a triplet or singlet configuration, with probability proportional to $\cos^2\theta$ and $\sin^2\theta$, respectively. Specifically, if $V = \sqrt{\sum_{\mathbf{k}} |V_{\mathbf{k}}|^2} \ll U_0$, the Kondo exchange, J_{eff}, can be found by second order perturbation theory:

$$\begin{aligned}\frac{J_{\text{eff}}}{2V^2} &= \langle \text{GS}, \uparrow|\, c^\dagger_{0\uparrow}\, \frac{1}{\mathcal{H} - E_{\text{GS}}}\, c_{0\downarrow}\,|\,\text{GS}, \downarrow\rangle \\ &\quad - \langle \text{GS}, \uparrow|\, c_{0\downarrow}\, \frac{1}{\mathcal{H} - E_{\text{GS}}}\, c^\dagger_{0\uparrow}\,|\,\text{GS}, \downarrow\rangle,\end{aligned} \tag{4}$$

where

$$\begin{aligned} c_{0\downarrow(\uparrow)}\,|\,\text{GS}, \downarrow(\uparrow)\rangle &= \mp\frac{\cos\theta}{\sqrt{3}}\ |\,t, 0\rangle - \sin\theta\ |\,s\rangle, \\ c^\dagger_{0\uparrow(\downarrow)}\,|\,\text{GS}, \downarrow(\uparrow)\rangle &= -\frac{\cos\theta}{\sqrt{3}}\, c^\dagger_{0\uparrow} c^\dagger_{0\downarrow}\,|\,t, 0\rangle \mp \sin\theta\, c^\dagger_{0\uparrow} c^\dagger_{0\downarrow}\,|\,s\rangle, \end{aligned}$$

and where

$$\begin{aligned} |\,t, 0\rangle &= \frac{1}{\sqrt{2}}\big(c^\dagger_{+1\uparrow} c^\dagger_{-1\downarrow} + c^\dagger_{+1\downarrow} c^\dagger_{-1\uparrow}\big)\,|\,0\rangle, \\ |\,s\rangle &= \frac{1}{\sqrt{2}}\big(c^\dagger_{+1\uparrow} c^\dagger_{-1\downarrow} - c^\dagger_{+1\downarrow} c^\dagger_{-1\uparrow}\big)\,|\,0\rangle, \end{aligned}$$

are the $S_z = 0$ component of the triplet state and the singlet state, respectively. It follows that

$$\begin{aligned}\frac{J_{\text{eff}}}{2V^2} &= -\frac{\cos^2\theta}{3}\,\langle t, 0\,|\,\mathcal{R}\,|\,t, 0\rangle + \sin^2\theta\,\langle s\,|\,\mathcal{R}\,|\,s\rangle \\ &\equiv -\frac{\cos^2\theta}{3}\,\gamma_t + \sin^2\theta\,\gamma_s,\end{aligned} \tag{5}$$

where the resolvent operator

$$\mathcal{R} = \frac{1}{\mathcal{H} - E_{\text{GS}}} + c_{0\downarrow} c_{0\uparrow}\, \frac{1}{\mathcal{H} - E_{\text{GS}}}\, c^\dagger_{0\uparrow} c^\dagger_{0\downarrow},$$

and $\gamma_s > \gamma_t > 0$, because the intermediate singlet state has lower energy than the triplet. The lead-dot exchange is therefore ferromagnetic if $\gamma_t\, \cos^2\theta > 3\,\gamma_s\, \sin^2\theta$, and antiferromagnetic in the opposite case, while $\gamma_t\, \cos^2\theta = 3\,\gamma_s\, \sin^2\theta$ actually identifies the transition between the two. We observe that, if inversion symmetry holds, $J_+ = J_-$, then $\theta = 0$ hence the lead-dot exchange is ferromagnetic, providing therefore a realization of the FKM. We expect that in a real device inversion symmetry will be generally broken; nevertheless there still is a good chance for ferromagnetism to survive in a wide region (by definition $\cos^2\theta \geq 3\sin^2\theta$, hence just because $\gamma_s > \gamma_t$ is it possible for the Kondo exchange to turn antiferromagnetic).

In conclusion, the set-up shown in fig. 1 seems indeed able to realize the much-sought FKM. Moreover, it suggests a simple way to study experimentally the transition from the FKM to the more conventional antiferromagnetic Kondo model, first described by Anderson, Yuval and Hamann [21], and expected to be of the BKT type. Indeed, changing the gate voltage ϵ_{+1} with respect to ϵ_{-1} drives the system further away from the inversion symmetric point, eventually turning the exchange from ferromagnetic to antiferromagnetic. We investigate this possibility by considering the Hamiltonian (1) in the simple case when $t_+ = t_- = t$, $U_0 = U_{+1} = U_{-1} = U$, and studying it as function of $\epsilon_{+1} = -\epsilon_{-1} = \delta\epsilon$ by means of NRG.[16–18] For simplicity we take a flat conduction-band density of states, $\rho(\epsilon) = \rho_0 = 1/2D$ when $\epsilon \in [-D, D]$ and zero otherwise, with the half-bandwidth D our unit of energy. Calculations employ a home-built NRG code, which implements as quantum numbers charge and the z-axis projection of the total spin. We use the value $\Lambda = 2$ for the discretization parameter of the conduction band, and keep 300 states per subspace, which roughly means 3500 total states per iteration. The spectral functions ($i = -1, 0, +1$)

$$\begin{aligned} A_i(\omega) &= \sum_{mn\sigma} |\langle m|c^\dagger_{i\sigma}|n\rangle|^2 \delta(\omega - \omega_{mn})\, \frac{\mathrm{e}^{-\beta E_m} + \mathrm{e}^{-\beta E_n}}{Z}, \\ Z &= \sum_n \mathrm{e}^{-\beta E_n}, \quad \beta = (k_B T)^{-1}, \quad \omega_{mn} = E_m - E_n, \end{aligned}$$

are computed through the patching technique,[22, 23] and delta-peaks are broadened in the form

$$\delta(\omega - \omega_{mn}) \to \frac{\mathrm{e}^{-b^2/4}}{b\,\omega_{mn}\sqrt{\pi}}\ \mathrm{e}^{-(\ln\omega - \ln\omega_{mn})^2/b^2},$$

with $b = 0.7$. The temperature is set by the length of the NRG chain and is almost zero, $T \sim 10^{-8} D$.

In fig. 2 we show the single-particle spectral density on the central dot, $A_0(\omega)$, as a function of the frequency

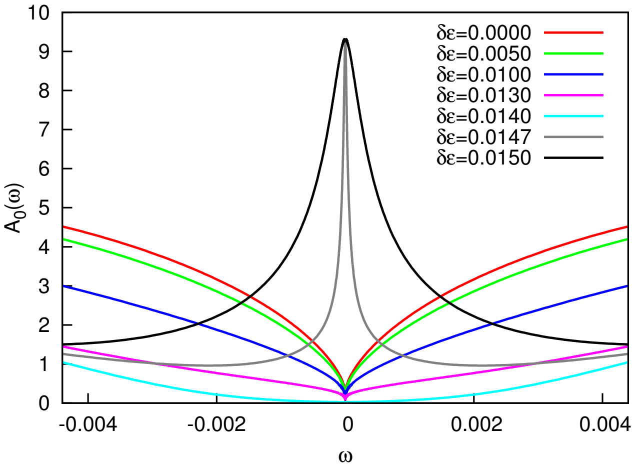

FIG. 2. (Color online) NRG spectral function $A_0(\omega)$ on dot 0 as a function of $\delta\epsilon$ for $U = 0.3$, $t = 0.03$, $\Gamma = 0.02\,\pi$ with a flat conduction band density of states of half-bandwidth $D = 1$. Note the transition from the ferromagnetic Kondo, signaled by a minimum of $A_0(\omega)$ at $\omega = 0$, to the regular, antiferromagnetic Kondo, where instead $A_0(\omega)$ is maximum at $\omega = 0$.

ω for different values of $\delta\epsilon$. $A_0(\omega = 0)$ is actually proportional to the zero-bias conductance,[24] while its behavior at small ω mimics that of the conductance at small bias. We note that for small $\delta\epsilon$, which corresponds to a ferromagnetic Kondo exchange, $J_{\rm eff} < 0$ in Eq. (5), $A_0(\omega = 0) = 0$; the zero-bias conductance vanishes and the zero-bias anomaly is inverted. This spectral function displays a logarithmic "dimple" at $\omega = 0$, associated with the $1/\ln^2\left(\omega/T_0\right)$ singularity typical of the FKM.[13] Here $T_0 \propto \sqrt{|J_{\rm eff}|}\,\exp\left(-1/\rho_0\,J_{\rm eff}\right)$ is an energy scale that actually diverges on approaching the BKT transition from the ferromagnetic side, i.e. $J_{\rm eff} \to 0$ from below.[13]

On the contrary, above a critical $\delta\epsilon_c$, $A_0(\omega = 0)$ suddenly jumps to a finite value; the conventional Abrikosov-Suhl spectral anomaly of the regular, antiferromagnetic Kondo model is recovered. Because of our choice of parameters, the Hamiltonian is particle-hole symmetric hence $A_0(\omega = 0)$ jumps from 0 to its unitary value $2/(\pi\Gamma)$ at the transition. Away from particle-hole symmetry, the jump still exists but will be smaller. The energy scale that controls the antiferromagnetic side, $J_{\rm eff} > 0$, is of course the Kondo temperature $T_K \propto \sqrt{J_{\rm eff}}\,\exp\left(-1/\rho_0\,J_{\rm eff}\right)$, usually defined as the half-width at half-maximum of $A_0(\omega)$, which vanishes on approaching the BKT transition, $J_{\rm eff} \to 0$ from above.

The standard, most reliable way to reveal the Kondo-like origin of a zero bias anomaly is by applying a magnetic field B. In the standard antiferromagnetic Kondo-effect, a magnetic field will split the Abrikosov-Suhl resonance only if sufficiently large, $g\mu_B B \gtrsim 0.5\,T_K$ [25]. This is indeed the case on the antiferromagnetic side of

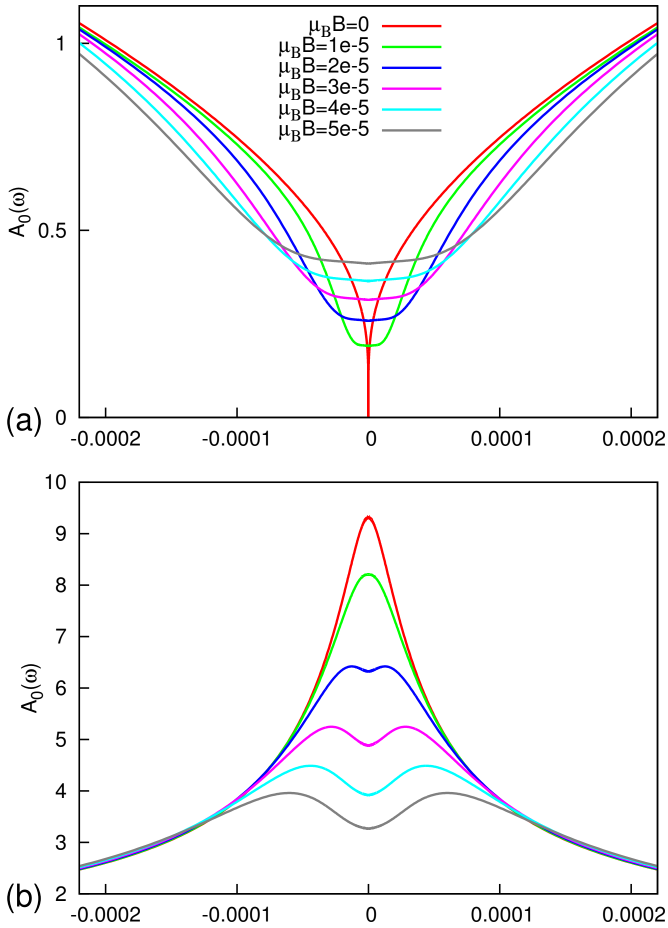

FIG. 3. (Color online) NRG spectral function $A_0(\omega)$ of the central dot 0, for increasing magnetic field B (we take $\mu_B = 1$ and $g = 2$, hence $2B$ is the Zeeman splitting) and the same parameters of Fig. 2. Panel (a) refers to $\delta\epsilon = 0$, while panel (b) to $\delta\epsilon = 0.0147$. In the ferromagnetic Kondo (FMK) regime, panel (a), the logarithmic dimple is immediately destroyed, and replaced by inelastic spin-flip excitations; in the antiferromagnetic (standard) Kondo regime, panel (b), where $T_K \simeq 6\times 10^{-5}$, the Abrikosov-Suhl resonance is only split by a sufficiently large field $2g\mu_B B \sim k_B T_K$.

the transition, $J_{\rm eff} > 0$, see panel (b) of fig. 3. On the contrary, on the ferromagnetic side, $J_{\rm eff} < 0$, panel (a), any magnetic field, however small, destroys the logarithmic dimple replacing it right away with a symmetric pair of inelastic spin-flip Zeeman excitations. In addition, $A_0(\omega = 0)$, hence the zero-bias conductance, increases with B at low temperature, contrary to the antiferromagnetic side, where it drops. We expect moreover that a finite temperature T will cutoff the logarithmic dimple at low frequency and raise up $A_0(\omega = 0) \sim 1/\ln^2(T/T_0)$, thus leading to an increase of zero-bias conductance, again unlike the regular antiferromagnetic Kondo effect.

In conclusion, we have shown that a three dot device, the central one contacted by metal leads, may provide

a realization of the ferromagnetic Kondo model. Gating of the lateral dots will in addition drive a Berezinskii-Kosterlitz-Thouless transition from ferromagnetic Kondo to regular, antiferromagnetic Kondo effect. The two phases should differ sharply in their zero-bias conductance anomaly, the ferromagnetic one being inverted and very differently modified by a magnetic field and by temperature.

More generally, our proposed system illustrates a generic mechanism leading to FKM, namely tunneling across one orbital in presence of other magnetic orbitals.This kind of situation could for example also be realized at selected surface adsorbed molecular radicals and detected in, e.g., STS or photoemission anomalies, an area where there is much active work. However, we should mention that, according to our calculations, the FKM anomalies are more visible when both U and the tunneling amplitude into the leads are larger than the inter-dot tunneling t, which might be hard to achieve in molecular radicals.

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